Using **attention-based neural networks** to enable **explainable drug sensitivity** prediction on **multimodal** data

Towards Explainable Anticancer Compound Sensitivity Prediction via Multimodal Attention-based Convolutional Encoders

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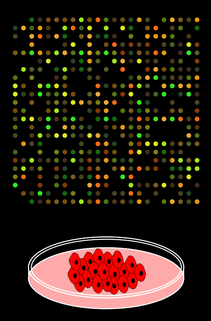
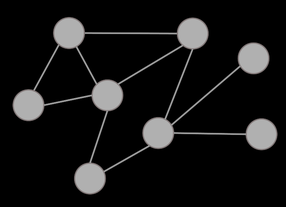
PaccMann tackles the challenging problem of drug sensitivity prediction adopting a holistic approach.
The model was trained on data from Genomics of Drug Sensitivity in Cancer (GDSC, `https://www.cancerrxgene.org/`)

SMILES

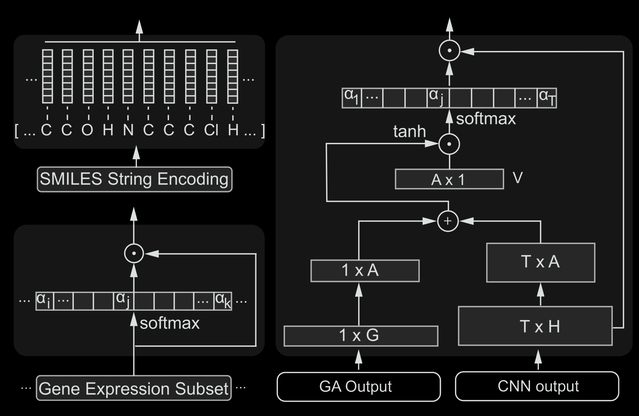
Gene expression

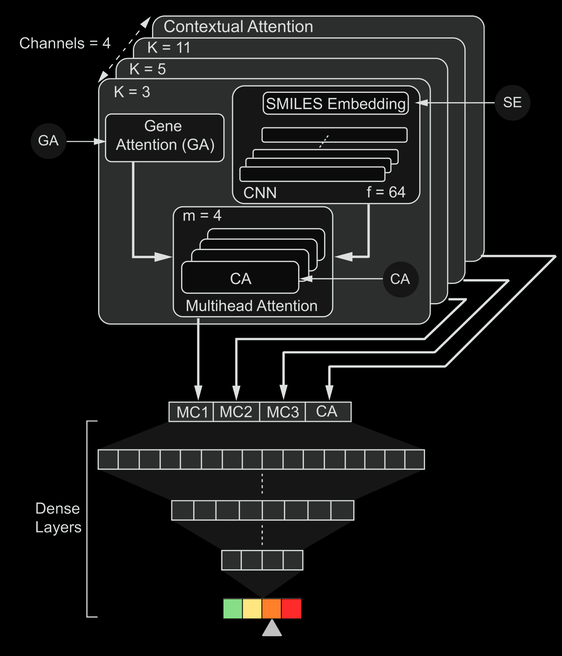


PPI



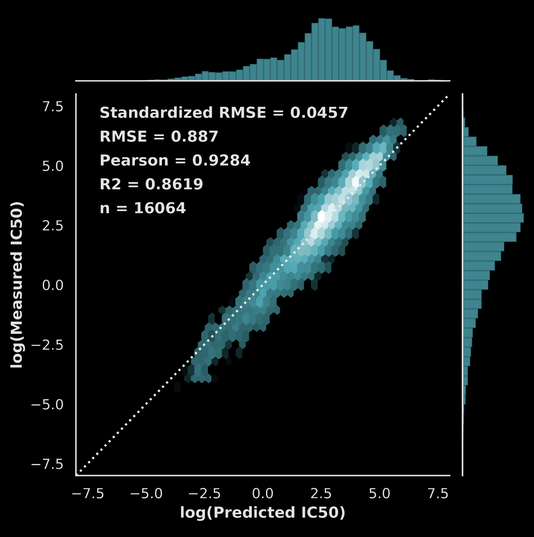
Gene expression and molecular structure are combined with multiple attention heads focusing on different scales





The model outperforms a baseline based on molecular fingerprints as well as different deep learning approaches, and accurately predicts drug sensitivity on unseen drug-cell line pairs

Encoder	Drug structure	Standardized RMSE Median ± IQR
Deep baseline (DNN)	Fingerprints	0.122 ± 0.010
Bidirectional recurrent (bRNN)	SMILES	0.119 ± 0.011
Stacked convolutional (SCNN)	SMILES	0.130 ± 0.006
Self-attention (SA)	SMILES	0.112* ± 0.009
Contextual attention (CA)	SMILES	0.110* ± 0.007
Multiscale convolutional attentive (MCA)	**SMILES**	**0.109* ± 0.009**
MCA (prediction averaging)	**SMILES**	**0.104** ± 0.005**



Try PaccMann

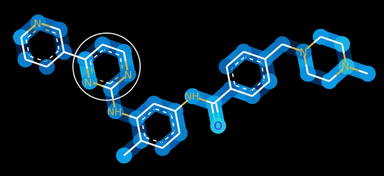
Web service
`https://ibm.biz/paccmann-aas`
GitHub
`https://github.com/drugilsberg/paccmann`

More info on PaccMann can be found in the WCB ICML 2019 paper
`https://ibm.biz/paccmann-paper`

The designed attention mechanism identifies relevant molecular substrcutures and highlights key genes for drug efficacy prediction

Masitinib

Imatinib



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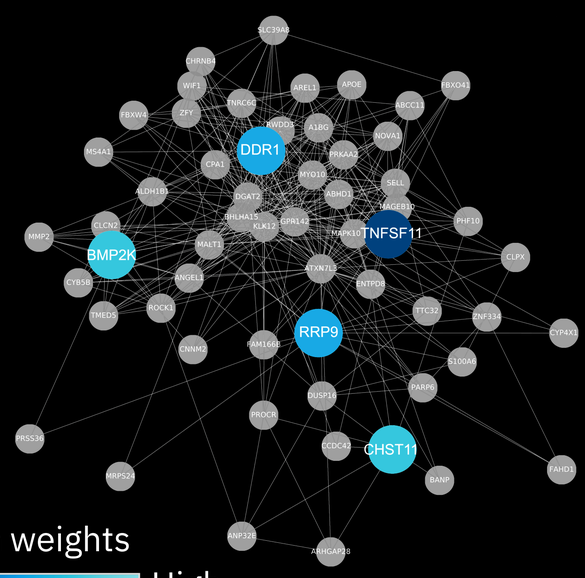

Attention weights
Low — High

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Prediction of **a**nti**c**ancer **c**ompound sensitivity with **m**ulti-modal **a**ttention-based **n**eural **n**etworks

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